<Bioinformatics Center> Bioknowledge Systems

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- Bioknowledge Systems -

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Scope of Research

Owing to continuous developments of high throughput experimental technologies, projects are going on not only to determine complete genome sequences of an increasing number of organisms, but also to analyze gene expression profiles both at the mRNA and protein levels and to catalog protein 3D structure families. Bioinformatics provides basic concepts as well as practical methods to go up from the molecular level to the cellular level, and eventually to still higher levels, to that of biological systems by analyzing complex interactions among building blocks and with dynamic environments. We have been developing such bioinformatics technologies and the KEGG system (http://www.genome.jp/kegg/), which is our attempt to uncover and utilize cellular functions through the reconstruction of protein interaction networks from genome information.

Research Activities (Year 2006)

Grants

Kanehisa M, Education and Research Organization for Genome Information Science, MEXT.

Kanehisa M, Knowledge Information Infrastructure for Genome Information Science, Kyoto University 21 st Century COE Program, MEXT.

KEGG DRUG Database

Chemical genomics is the next stage of post-genomic analysis. Drugs, environmental substances and various chemical compounds contribute to the fluctuation of bio-system. Therefore, chemical genomic analysis would require the investigation of relationships between genomes and their external compounds.

These relationships between bio-systems and external compounds include interaction between cell and drug. At present, discovery of new drugs with desired physico-chemical and biological properties has been a long-standing challenge in pharmaceutical researches. Most of current drugs have evolved from original compounds found by chance through empirical screening. In the process of this evolution, continuous modifications have been made in an empirical manner to optimize targets to new molecules with better efficacy. It is possible to extract such a manner from a lot of data.

The KEGG DRUG database is a new addition to the KEGG LIGAND database, which contains the chemical structures of drugs and additional information such as therapeutic categories and target molecules. In particular, the KEGG DRUG Structure Map graphically illustrates our knowledge on drug development on the basis of chronology, targets and skeletons. This useful information must help new drug discovery.

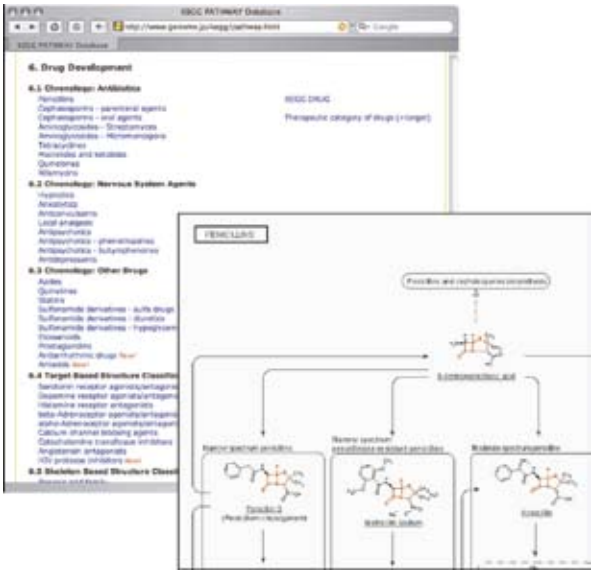

Figure 1. The KEGG DRUG Structure Map.

GENIES: Gene Network Inference Engine Based on Supervised Analysis

The GENIES is a newly developed system to infer a global gene network consisting of functional associations between genes based on various genomic information and high-throughput experimental data (e.g., gene positions, phylogenetic profiles, gene expression profiles and protein intracellular localization) in the framework of supervised network inference. Figure 2 shows an illustration of the procedure in the GENEIS. The GENIES enables us to predict unknown functional relationships between genes, and fill in the pathway holes by selecting candidate genes coding for missing enzymes in metabolic pathways.

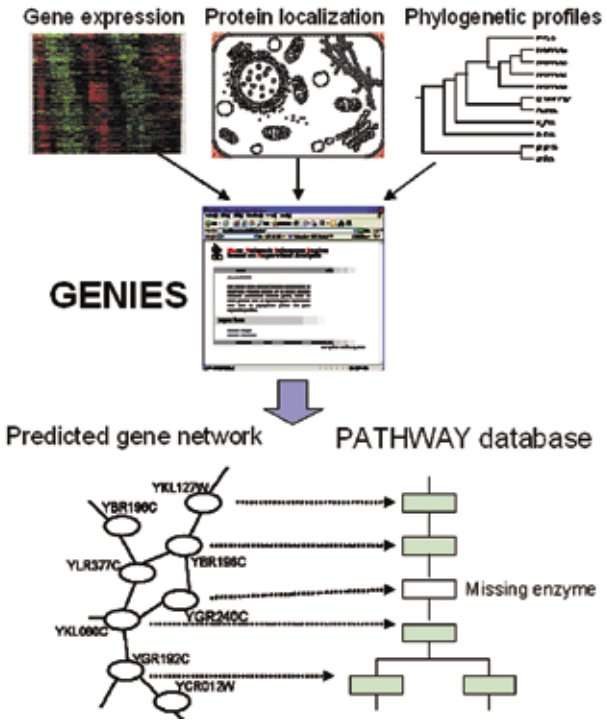

Figure 2. Various genome-wide datasets are used for predicting a global gene network.

Kanehisa M, Backbone Database for Analysis of the Biological Systems and Environment, Grants-in-Aid for Scientific Research on Priority Areas, MEXT.

Kanehisa M, Deciphering Systemic Biological Functions by Integration of Genomic and Environmental Information, Bioinformatics Research and Development, JST.

Kanehisa M, Integration of Genomics and Chemistry in Glycome Informatics, NIH, USA.

Goto S, Probing the *Plasmodium falciparum* Genome, Contact Research, JST.